

科目：物理化學 適用：應化所

考生注意：

1. 依次序作答，只要標明題號，不必抄題。
2. 答案必須寫在答案卷上，否則不予計分。
3. 限用藍、黑色筆作答；試題須隨卷繳回。

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Physical Constant

Symbol, Value and Unit

Gas constant:  $R = 0.08206 \text{ atm dm}^3 \text{ mole}^{-1} \text{ K}^{-1} = 8.315 \text{ J mole}^{-1} \text{ K}^{-1}$ Note:  $I_n = \int_0^\infty e^{-ar} r^n dr = \frac{n!}{a^{n+1}}$ ,  $\ln 2 = 0.6931$ 

1. (30%) For an enzyme catalysis reaction  $E + S \xrightleftharpoons[k_{-1}]{k_1} ES \xrightleftharpoons[k_{-2}]{k_2} E + P$ , where E is the

enzyme with initial concentration  $[E]_0$ , S is the substrate with initial concentration  $[S]_0$ , ES is the enzyme-substrate complex, and P is the product.  $k_1$ ,  $k_2$ ,  $k_{-1}$  and  $k_{-2}$  are the rate constants. Assume  $K_i$  is the equilibrium constant of the first reaction and  $k_2$  is evaluated as  $k_i$  at temperature  $T_i$ , and  $K_j$  is the equilibrium constant of the first reaction and  $k_2$  is evaluated as  $k_j$  at temperature  $T_j$ . (a) Using steady-state approximation, find the initial rate of the reaction in terms of rate constants  $k_1$ ,  $k_2$ ,  $k_{-1}$ ,  $[S]_0$  and  $[E]_0$ . (b) Express the standard thermodynamic enthalpy ( $\Delta H^\circ$ ) for the formation of ES and the activation energy  $E_a$  for  $k_2$  in terms of  $k_i$ ,  $T_i$ ,  $K_i$ ,  $k_j$ ,  $T_j$ , and  $K_j$ .

2. (30%) The wavefunction of 1s orbital for the hydrogen atom is

$$\Psi_{1s} = C \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

(a) Find the value of C that normalizes the orbital (b)

Calculate the average distance  $\langle r \rangle$  between the nucleus and electron in terms of  $a_0$ . (c) Calculate the most probable distance  $r$  to find the electron in terms of  $a_0$ .

3. (10%) The Hamiltonian for "the particle in a box problem" along the x direction

is defined as  $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ . Apply the variation method with trial function

$$\Psi = \sin\left(\frac{\pi x}{a}\right)$$

to calculate an energy for a particle of mass  $m$  moving in an

one-dimensional box of length  $a$ .

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4. (10%) Consider a three-dimensional cubic box of length  $d$ , containing eight non-interacting electrons with each mass as  $m$ . Given that the energy levels for electrons in three-dimensional box are  $E_{nml} = (n^2 + m^2 + l^2)(h^2/8md^2)$ , where  $n$ ,  $m$ , and  $l$  are quantum number. (a) Calculate the energy of the ground state of this system in terms of  $h$ ,  $d$ , and  $m$ . (b) Calculate the energy of the first excited state of this system in terms of  $h$ ,  $d$ , and  $m$ .
5. (20%) A sample of 1.00 mol of a monoatomic perfect gas, initially at 298 K and 10 liters, is expanded isothermally and reversibly, to a final volume of 20 liters with surroundings maintained at 298 K. Calculate  $\Delta S$ ,  $\Delta U$ ,  $\Delta H$ ,  $\Delta A$ , and  $\Delta G$  for this case.

試題